Machine Learning 1

Lecture 10.2 - Unsupervised Learning
Principal Component Analysis -
Reconstruction Error Minimization

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(Bishop 12.1.2, 12.1.3)

Slide credits: Rianne van den Berg

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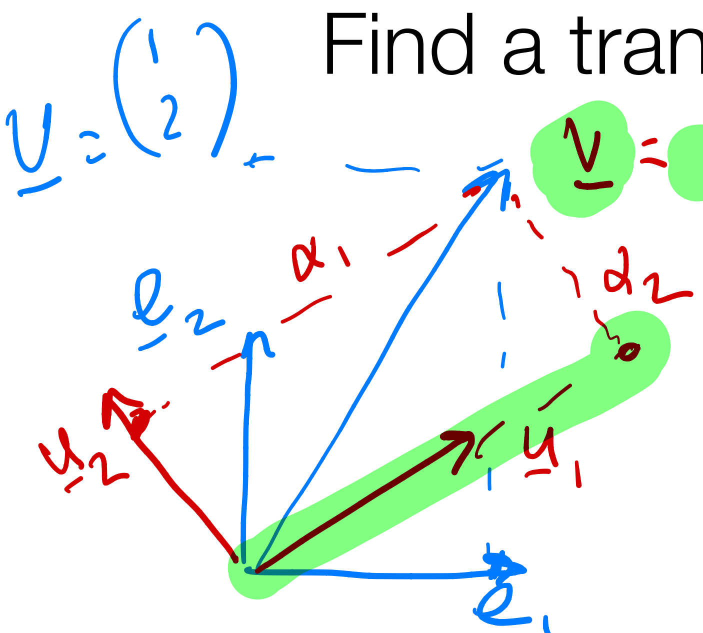
PCA via minimal reconstruction error

- Same method, alternative view to the maximal variance viewpoint

- PCA can be obtain by minimizing the reconstruction error. Find a transformation that minimizes:



$\underline{v} = \alpha_1 \underline{u}_1 + \alpha_2 u_2$

$$\frac{1}{N}\sum_{n=1}^{N} \|\mathbf{x}_n - \tilde{\mathbf{x}}_n\|$$

$\underline{z}_n$

basis $\mathbb{R}^{D \times M}$

$\tilde{x}_n = U_M \underline{z}_n + \underline{\bar{x}}$

latent variable / basis coefs

$\mathbb{R}^M$

Before we focussed on embedding

$\underline{z}_n = U_M^T \underline{x}_n$

- Represent the points in a different orthonormal basis (unknown for now):

$$\{\mathbf{u}_i : \mathbf{u}_i^T \mathbf{u}_i = 1\}_{i=1}^{D} \qquad \mathbf{u}_i^T \mathbf{u}_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

PCA via minimal reconstruction error

- In the new basis $$\mathbf{x}_n = \sum_{i=1}^{D} \alpha_{ni} \mathbf{u}_i$$

property of orthonormal basis

- The coefficients are found by multiplying with $\mathbf{u}_j^T$ on both sides:

$$\alpha_{ni} = \mathbf{x}_n^T \mathbf{u}_i$$

- Therefore… we get the projection onto the new basis:

$$\mathbf{x}_n = \sum_{i=1}^{D} \underbrace{(\mathbf{x}_n^T \mathbf{u}_i)}_{\alpha_{ni}} \underline{\mathbf{u}_i}$$

- For reconstruction, we use the first M elements of the basis and a shared offset for the remaining dimensions

$$\tilde{\mathbf{x}}_n = \sum_{i=1}^{M} \underbrace{(\mathbf{x}_n^T \mathbf{u}_i)}_{z_{ni}} \mathbf{u}_i + \sum_{i=M+1}^{D} b_i \mathbf{u}_i$$

shared for all data points

PCA via minimal reconstruction error

- The difference/error is then given by

first M components cancel out

$$\mathbf{x}_n - \tilde{\mathbf{x}}_n = \underbrace{\sum_{i=1}^{D} (\mathbf{x}_n^T \mathbf{u}_i)\, \mathbf{u}_i}_{x_n} - \underbrace{\sum_{i=1}^{M} (\mathbf{x}_n^T \mathbf{u}_i)\, \mathbf{u}_i - \sum_{i=M+1}^{D} b_i\, \mathbf{u}_i}_{\tilde{x}_n}$$

$$= \sum_{i=M+1}^{D} (\mathbf{x}_n^T \mathbf{u}_i)\, \mathbf{u}_i - \sum_{i=M+1}^{D} b_i\, \mathbf{u}_i$$

$$= \sum_{i=M+1}^{D} (\mathbf{x}_n^T \mathbf{u}_i)\, \mathbf{u}_i - b_i\, \mathbf{u}_i$$

PCA via minimal reconstruction error

- We have to minimize for both $\mathbf{u}_i$ and b_i

$$\frac{1}{N}\sum_{n=1}^{N}\|\mathbf{x}_n - \tilde{\mathbf{x}}_n\|^2 = \frac{1}{N}\sum_{n=1}^{N}\left\| \sum_{i=M+1}^{D} (\mathbf{x}_n^T\mathbf{u}_i)\,\mathbf{u}_i - b_i\,\mathbf{u}_i \right\|^2$$

- Solution for b_i is given by $b_i = \bar{x}^T\mathbf{u}_i$

- We are left to solve for $\mathbf{u}_i$, minimizing

$$\frac{1}{N}\sum_{n=1}^{N}\left\| \sum_{i=M+1}^{D} ((\mathbf{x}_n - \tilde{\mathbf{x}})^T\mathbf{u}_i)\,\mathbf{u}_i \right\|^2$$

PCA via minimal reconstruction error

$$\frac{1}{N}\sum_{n=1}^{N}\left\|\sum_{i=M+1}^{D}((\mathbf{x}_n-\tilde{\mathbf{x}})^T\mathbf{u}_i)\,\mathbf{u}_i\right\|^2$$

expand square

$$=\frac{1}{N}\sum_{n=1}^{N}\left(\sum_{i=M+1}^{D}\underbrace{((\mathbf{x}_n-\tilde{\mathbf{x}})^T\mathbf{u}_i)}_{\text{scalar}}\,\underbrace{\mathbf{u}_i}_{\text{vector}}\right)^T\left(\sum_{j=M+1}^{D}((\mathbf{x}_n-\tilde{\mathbf{x}})^T\mathbf{u}_j)\,\mathbf{u}_j\right)$$

$a^Tb = b^Ta$

$$=\frac{1}{N}\sum_{n=1}^{N}\sum_{i=M+1}^{D}\cancel{\sum_{j=M+1}^{D}}((\mathbf{x}_n-\tilde{\mathbf{x}})^T\mathbf{u}_i)\,\underbrace{\mathbf{u}_i^T\,\mathbf{u}_j}_{0 \text{ for all } i\neq j}((\mathbf{x}_n-\tilde{\mathbf{x}})^T\,\mathbf{u}_j)$$

$$=\frac{1}{N}\sum_{n=1}^{N}\sum_{i=M+1}^{D}\mathbf{u}_i^T(\mathbf{x}_n-\tilde{\mathbf{x}})(\mathbf{x}_n-\tilde{\mathbf{x}})^T\mathbf{u}_i=\sum_{i=M+1}^{D}\mathbf{u}_i^T\,\mathbf{S}\,\mathbf{u}_i$$

PCA via minimal reconstruction error

- We got: $\frac{1}{N}\sum_{n=1}^{N}||\mathbf{x}_n - \tilde{\mathbf{x}}_n||^2 = \sum_{i=M+1}^{D} \mathbf{u}_i^T \mathbf{S}\, \mathbf{u}_i = \sum_{i=M+1}^{D} \lambda_i$

- Solve for $\mathbf{u}_i$ under constraint $\mathbf{u}_i^T \mathbf{u}_i = 1$ (else we get $\mathbf{u}_i = \mathbf{0}$)

- Method of Langrange multipliers -> Solve eigensystem

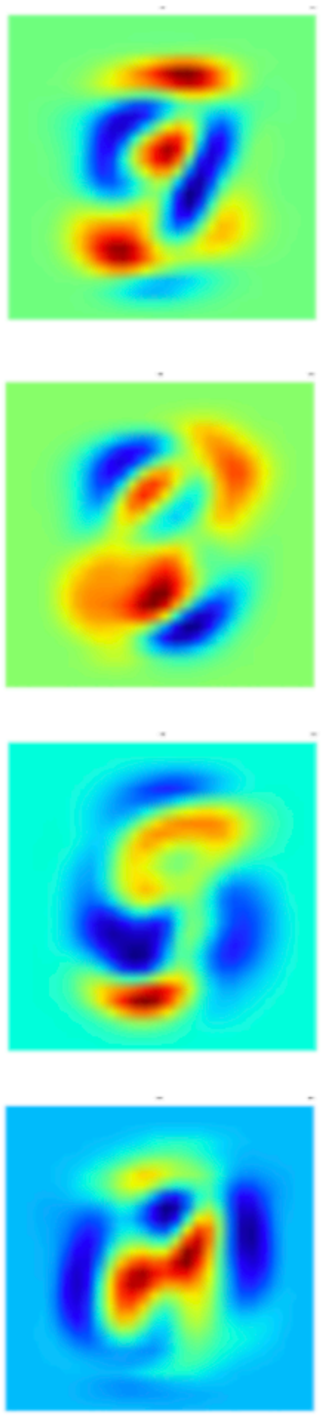
$$\Longrightarrow \mathbf{S}\,\underline{u}_i = \lambda_i \underline{u}_i$$

- Find the largest M eigenvectors and values, such that the remaining $(D - M)$ are the smallest

$$\boxed{\textbf{min reconstruction error = max projected variance}}$$

Applications: compression (MNIST)

Eigenvectors:



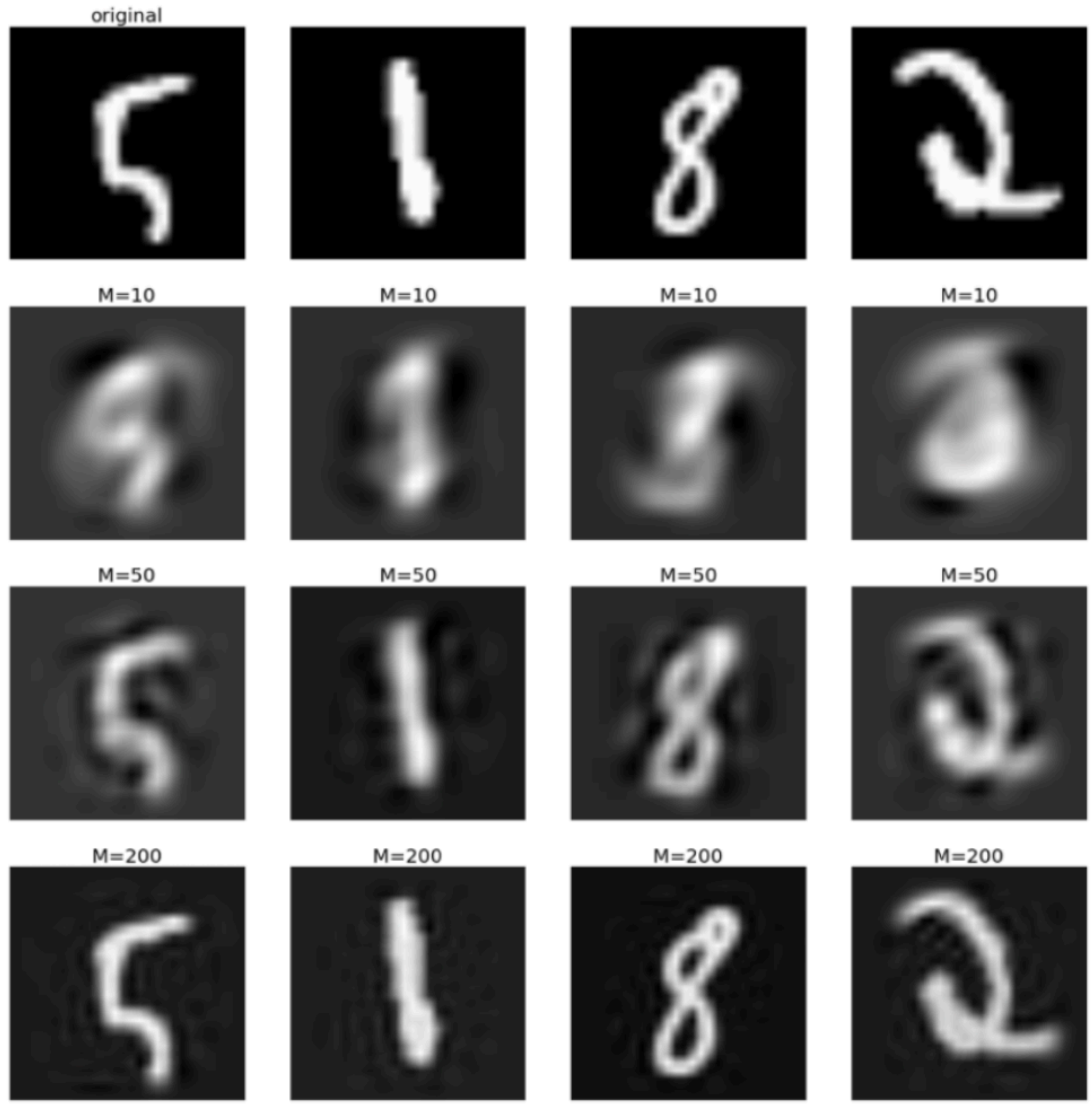
$\boldsymbol{u}_1$

$\boldsymbol{u}_2$

$\boldsymbol{u}_3$

$\boldsymbol{u}_4$

Reconstructions: $\tilde{\mathbf{x}} = \mathbf{U}_M \mathbf{z} + \bar{\mathbf{x}}$



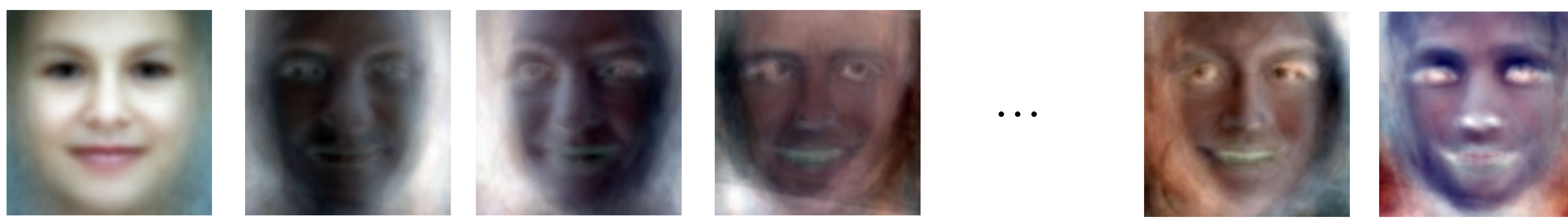
Applications: compression (eigenfaces/UTKFace)

Dataset: 

Task: Compress image

Method: Expand along principle components (PCA)

Mean $\bar{\mathbf{x}}$ $\mathbf{u}_1$ $\mathbf{u}_2$ $\mathbf{u}_3$ …



Result:

Original

$$\approx \bar{\mathbf{x}} + \sum_{i=1}^{M} z_{ni}\mathbf{u}_i$$

M=1 *M=10* *M=50* *M=150*